Appendix A: Calculations for Data Quality Assessment (sec. 4-5)

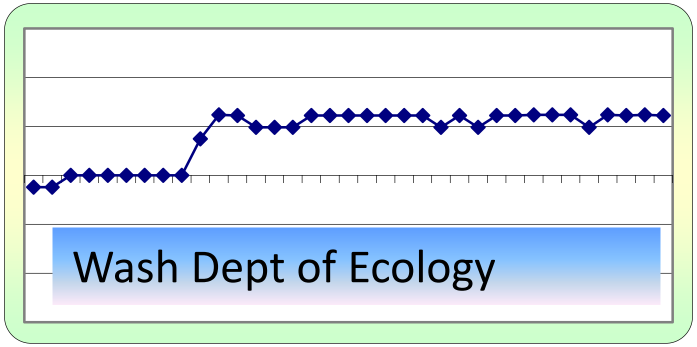
aka

<u>What Is Reality</u>?

- **1-pt QC check statistics**
- **Precision calcs**
- **Bias calcs**

Stats are designed to show us how far from the TRUTH we might be.

- ***Measurement Error***
  - Presented as a fraction of the "truth" (e.g., 10% off)
- ***Precision***
  - Random error
  - "wiggle" inherent in system
  - Estimated by (1) repeated measurements of "known," and/or (2) side-by-side measurements of the same thing
  - Some imprecision is unavoidable
- ***Bias***
  - Systematic error
  - "jump" consistently high or low
  - bias can be eliminated (in theory)

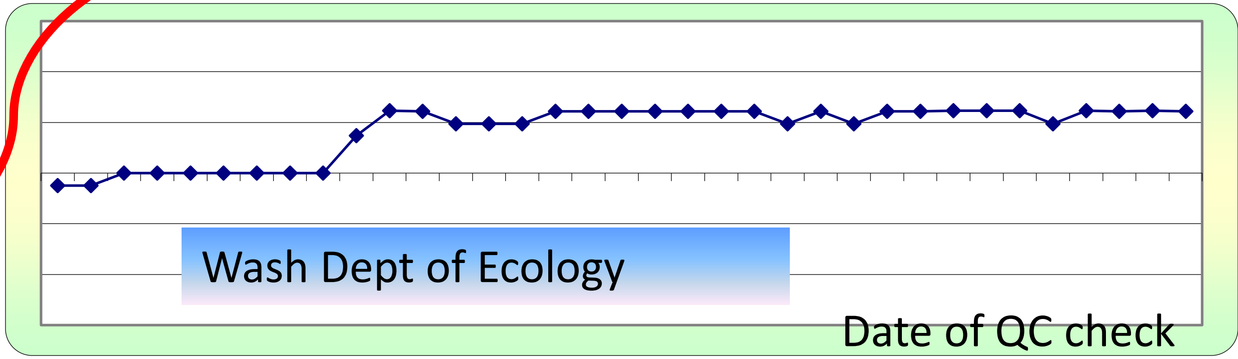


1-pt QC 0^3 check data, in AQS:

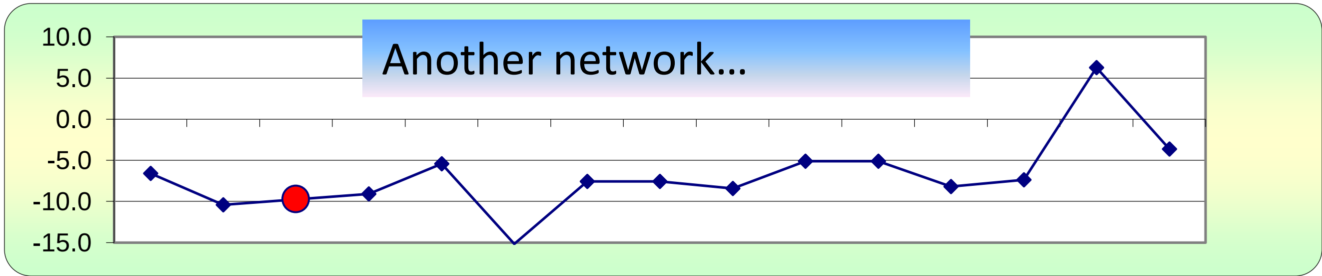
SITE 20	
Meas Val (Y)	Audit (known) Val (X)
85.1	91.1
81.6	91.1
83.4	92.4
84	92.4
87.4	92.4
78.4	92.4
85.4	92.4
85.4	92.4
80.6	88
83.5	88
83.5	88
80.8	88
81.5	88
93.5	88
84.8	88

d-sub-i = d_i = diff/known

- Routine QC checks used to estimate BOTH
- <u>Both</u> come from **d-sub-i**
- Bias
- Precision



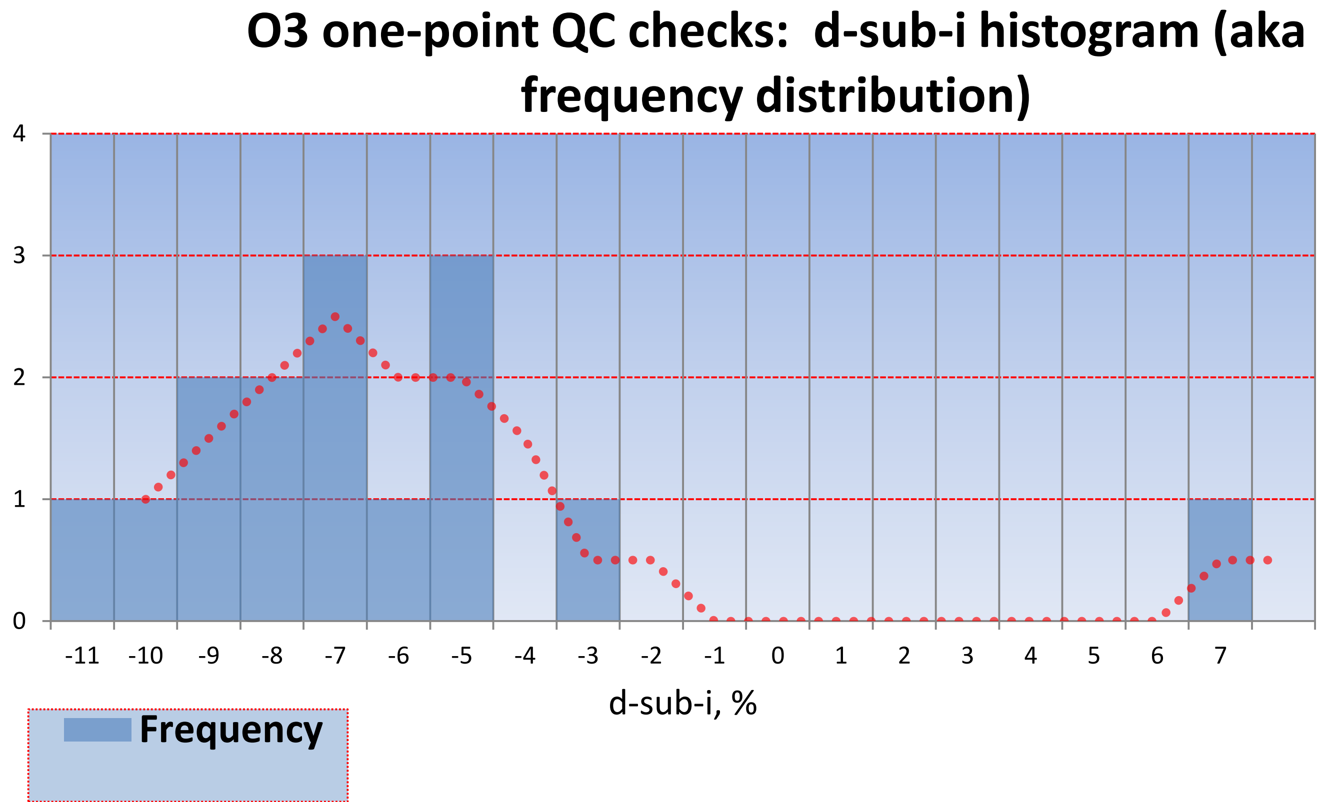
- sometimes it's obvious
- Sometimes it's not:



Meas Val (Y)	Audit Val (X)	d-sub-i
85.1	91.1	-7
81.6	91.1	-10
83.4	92.4	-10
84	92.4	-9
87.4	92.4	-5
78.4	92.4	-15
85.4	92.4	-8
85.4	92.4	-8
80.6	88	-8
83.5	88	-5
83.5	88	-5
80.8	88	-8
81.5	88	-7
93.5	88	6
84.8	88	-4

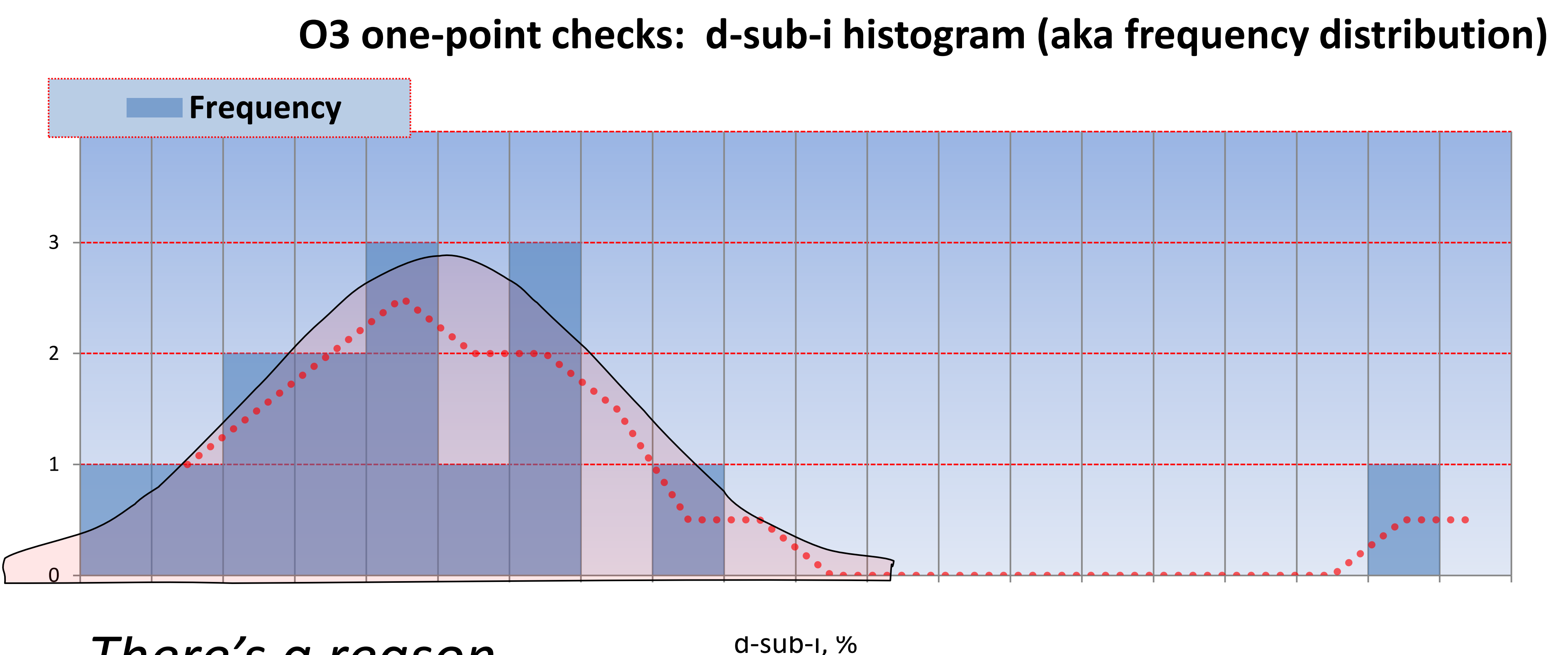
- d-sub-i values represent:
  - All of the measurements' error during that day, week, month, quarter
    - The QC checks are supposed to be "randomized" so that they are a sample, or subset, of the whole universe of possible QC checks (the population), and then represent the population of QC checks you could do at any time
  - As a proportion of the "truth," so "truth" is always on the bottom (diff/known; so error is quantified as a fraction of the truth so we can imagine it, e.g., 10%)
  - "error" = distance from truth at that moment

Meas Val (Y)	Audit Val (X)	d-sub-i
85.1	91.1	-7
81.6	91.1	-10
83.4	92.4	-10
84	92.4	-9
87.4	92.4	-5
78.4	92.4	-15
85.4	92.4	-8
85.4	92.4	-8
80.6	88	-8
83.5	88	-5
83.5	88	-5
80.8	88	-8
81.5	88	-7
93.5	88	6
84.8	88	-4



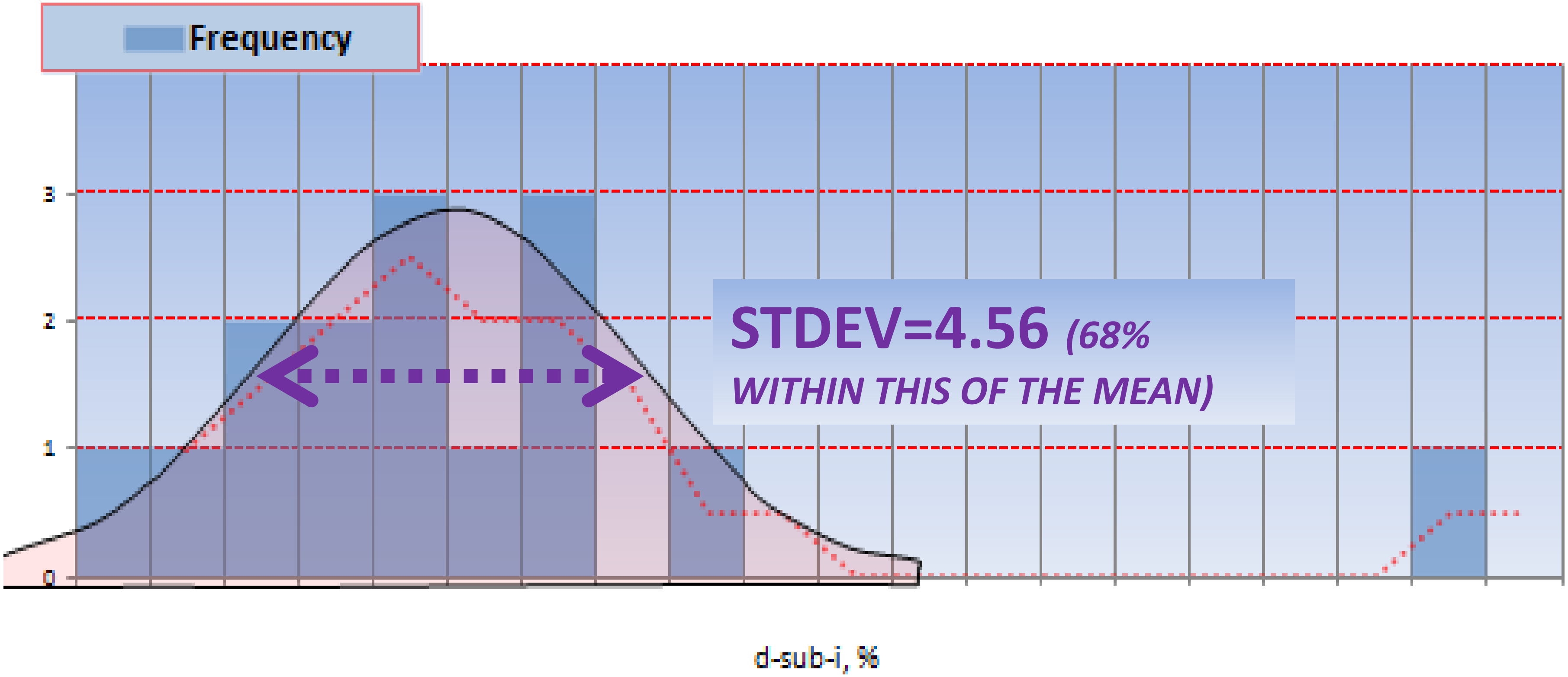
How can we apply these results to get bias and precision for ALL our measurements of ozone with this analyzer during this time period?

We assume that these results, <u>and their distribution</u>, is representative of all the QC checks we could have done:

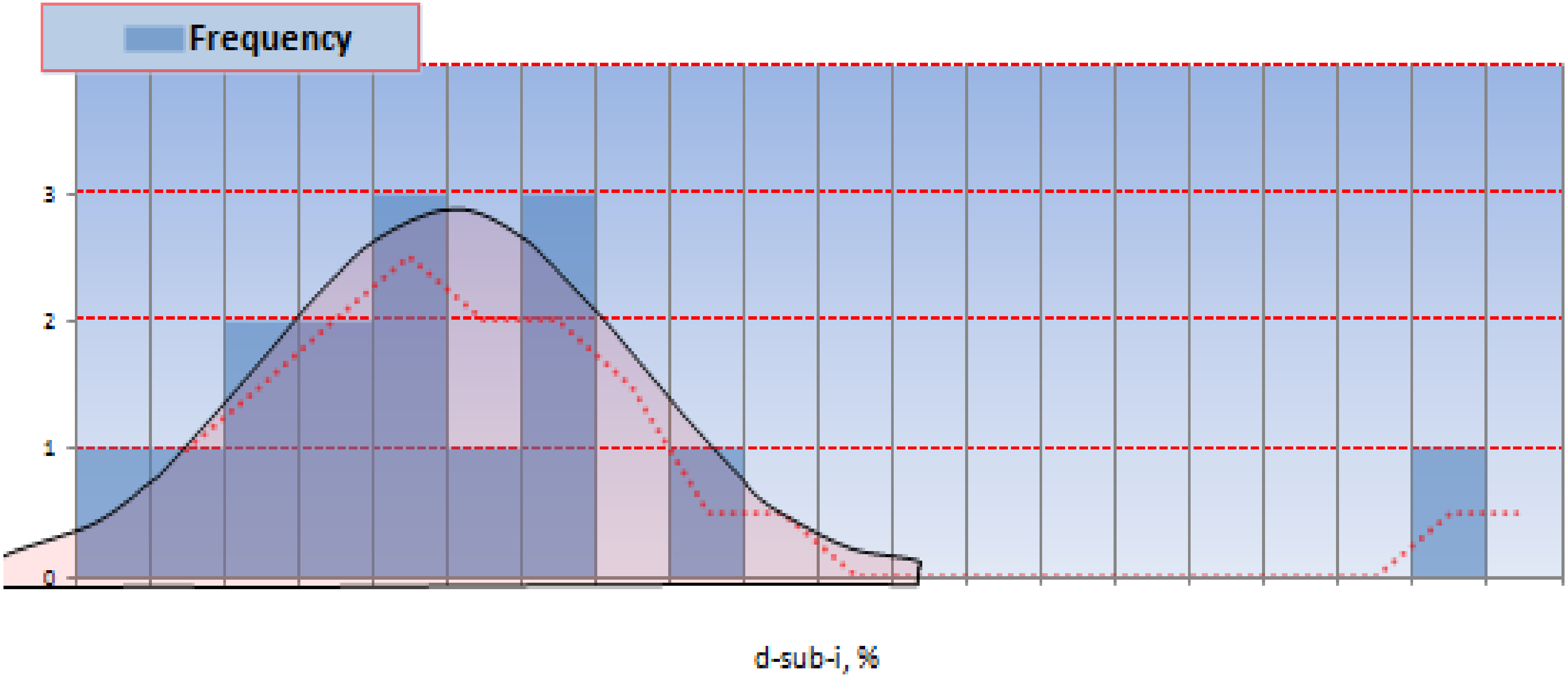


There's a reason no x-axis units

The goal for acceptable measurement uncertainty is defined for O3 precision as an upper 90 percent confidence limit for the coefficient variation (CV) of 7%



- But we do not care about the low-imprecision tail
- Only care about the <u>extreme</u> tail of high imprecision
- Want to be able to say “90% confident that your precision is less than this value”

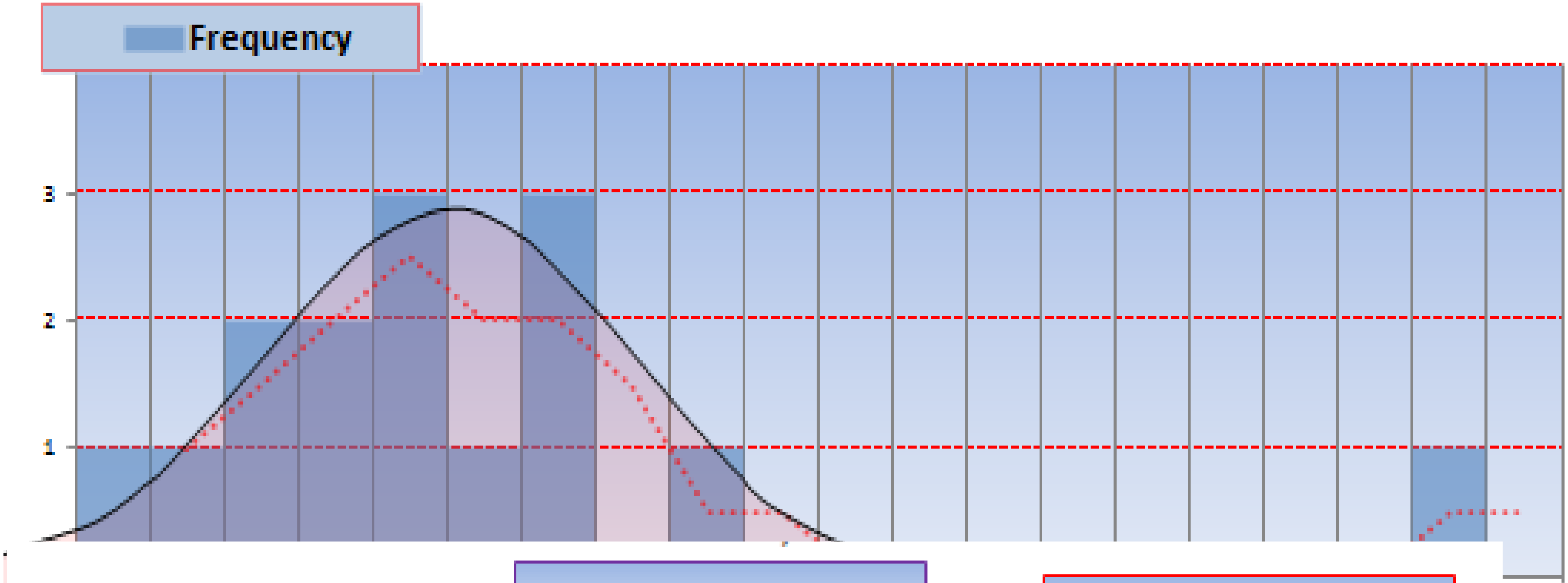


STDEV=4.56

10% upper tail

CFR eq'n 2:

$$Precision\_Estimate = \sqrt{\frac{n \bullet \sum_{i=1}^{n} d_i^2 - (\sum_{i=1}^{n} d_i)^2}{n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$



STDEV=4.56

10% upper tail

$$Precision\_Estimate = \sqrt{\frac{n \bullet \sum_{i-1}^{n} d_i^2 - (\sum_{i-1}^{n} d_i)^2}{n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

chi-sqrd(90%) = CHIINV(0.9,n) = 7.79

then 4.56 x SQRT(n-1/7.79) = 6.11 %

Use the DASC Tool to Understand Your QC Checks and Audit Results (like EPA does)

- Calculations of measurement uncertainty are carried out by EPA, *and* PQAOs should report the data for all measurement quality checks
- YOU do these calculations and charts easily, and save yourself time, money, and embarrassment

We will review each in both the DASC tool and the AMP256 report

First, what is the DASC tool?

- DASC tool was produced specifically for us to calculate the data assessment statistics in CFR in AMTIC Quality Indicator Assessment Reports (AMP256)
- http://www.epa.gov/ttn/amtic/qareport.html
- Easy way to explain and calculate data assessment statistics in CFR
- Excel spreadsheet
- Matches AMP256 (by site)
- Each equation is numbered and matches the numbers in CFR

DASC Tool:

O_3 Assessments

site 20		Pollutant type: O_3				
eas Val	it Val	d (Eqn. 1)	n Percen	d^2	|d|	$\|d\|^2$
85.1	91.1	-6.586	-8.750	43.378	6.586	43.378
81.6	91.1	-10.428	n Percen	108.745	10.428	108.745
83.4	92.4	-9.740	-5.262	94.873	9.740	94.873
84	92.4	-9.091		82.645	9.091	82.645
87.4	92.4	-5.411		29.282	5.411	29.282
78.4	92.4	-15.152		229.568	15.152	229.568
85.4	92.4	-7.576		57.392	7.576	57.392
85.4	92.4	-7.576		57.392	7.576	57.392
80.6	88	-8.409		70.713	8.409	70.713
83.5	88	-5.114		26.149	5.114	26.149
83.5	88	-5.114		26.149	5.114	26.149
80.8	88	-8.182		66.942	8.182	66.942
81.5	88	-7.386		54.558	7.386	54.558
93.5	88	6.250		39.063	6.250	39.063
84.8	88	-3.636		13.223	3.636	13.223

CV_{ub} (%)			Bias (%)	
n	S_d	S_{d2}	$\Sigma\|d\|$	"AB" (Eqn 4)
15	4.557	52.464	115.651	7.710
n-1	Σd	Σd^2	$\Sigma\|d\|^2$	"AS" (Eqn 5)
14	-103.151	1000.072	1000.072	2.783

Bias (%) (Eqn 3)	Both Signs Positive
8.98	FALSE
Signed Bias (%)	Both Signs Negative
-8.98	TRUE

CV (%) (Eqn 2)
6.11

Upper Probability Limit	Lower Probability Limit
2.06	-15.81

Return to Main Menu

Print Worksheet

Precision in DASC = cell i13 = 6.11%

O_3 Assessments

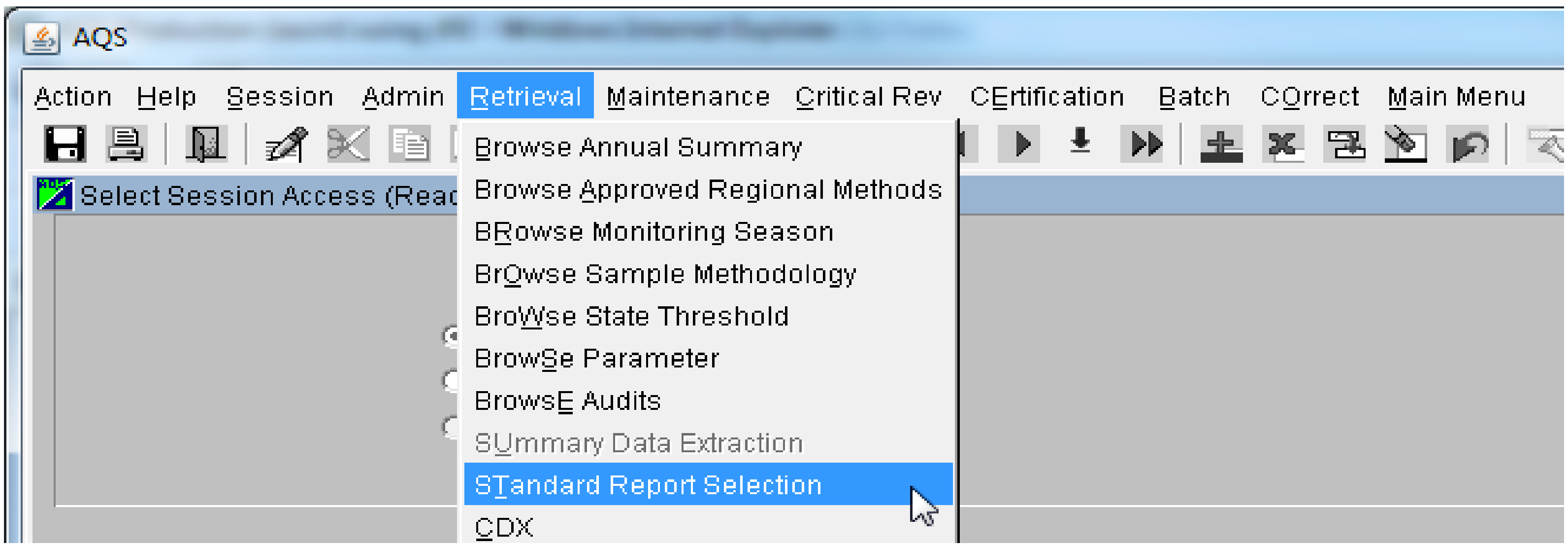
site 20		Pollutant type: O_3
Meas Val (Y)	Audit Val (X)	d (Eqn. 1)
85.1	91.1	-6.586
81.6	91.1	-10.428
83.4	92.4	-9.740
84	92.4	-9.091
87.4	92.4	-5.411
78.4	92.4	-15.152
85.4	92.4	-7.576
85.4	92.4	-7.576
80.6	88	-8.409
83.5	88	-5.114
83.5	88	-5.114
80.8	88	-8.182
81.5	88	
93.5	88	
84.8	88	

CV (%) (Eqn 2)
6.11

$$\Pr ecision\_Estimate = \sqrt{\frac{n \bullet \sum_{i=1}^{n} d_i^2 - (\sum_{i=1}^{n} d_i)^2}{n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

AMP256-Data Quality Indicators Report

- AQS Standard Report to Compute the Statistics Outlined on 40 CFR Part 58 Appendix A
- Part of the Annual Certification Process to Verify Submission of QA and routine Data to AQS



- **CORRESPONDS to what you can calculate in the DASC spreadsheet, as we will see.**

Does our 6.1% match AMP256?

DATA QUALITY INDICATOR REPORT

One Point Quality Control

Jun. 16, 2014

PQAO: Virginia I

App A? Y

POC	MT	Begin Date	End Date	# Required	# Observation	% Complete	CV UB	Bias UB
1	S	01-APR-12	31-OCT-12	15	15	100	6.11	- 8.98

- 90% Confidence Upper Bound of precision is 6.1%
- "There is a 90% chance that our precision will not be greater than 6.1%"
- Same as YOU can calculate any time using the DASC

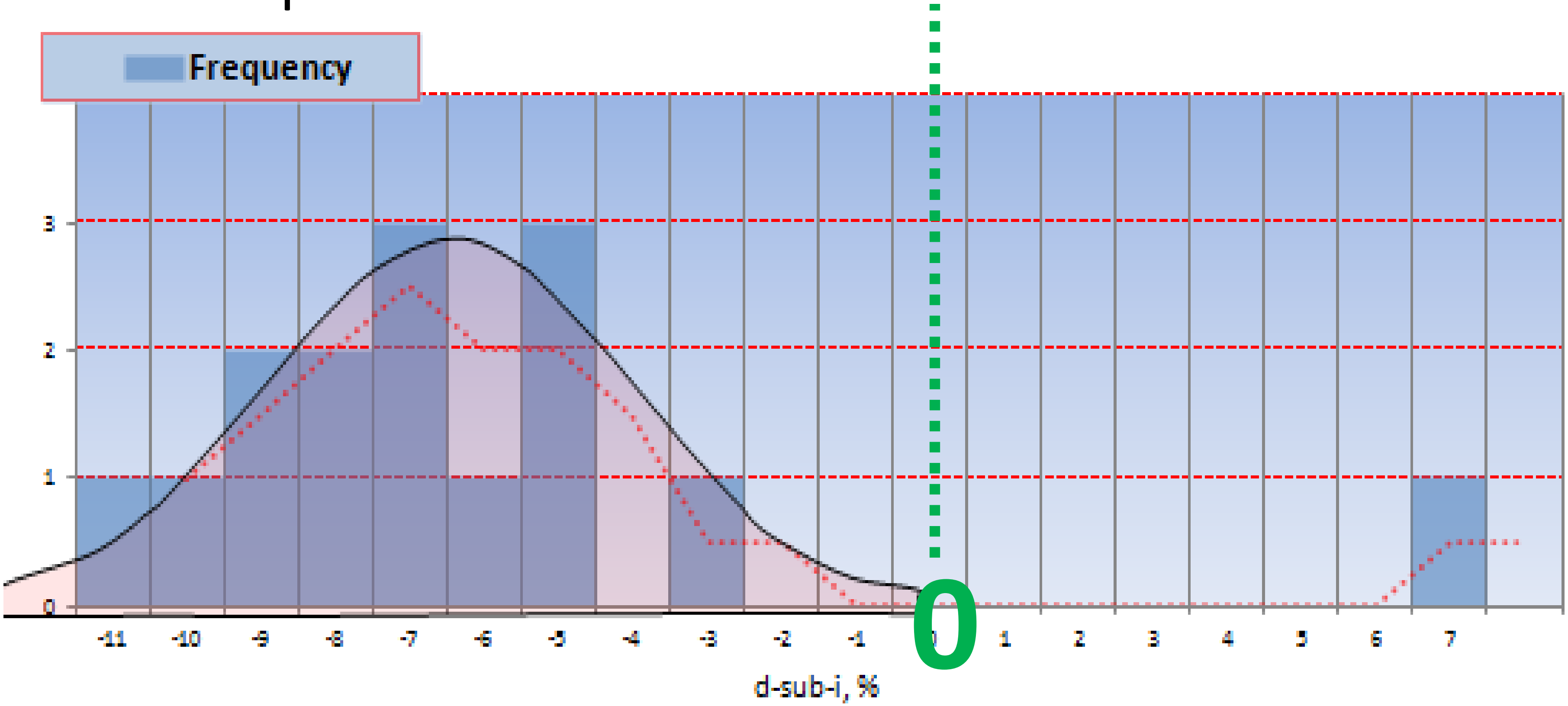
Summary of precision:

- Calculated from routine QC checks $\mathbf{d_i}$
- Overall upper bound of CV calculated from $\mathbf{d_i}$
- you can be **90% sure that your true precision is less than** this "upper bound of the CV" (eq'n 2)

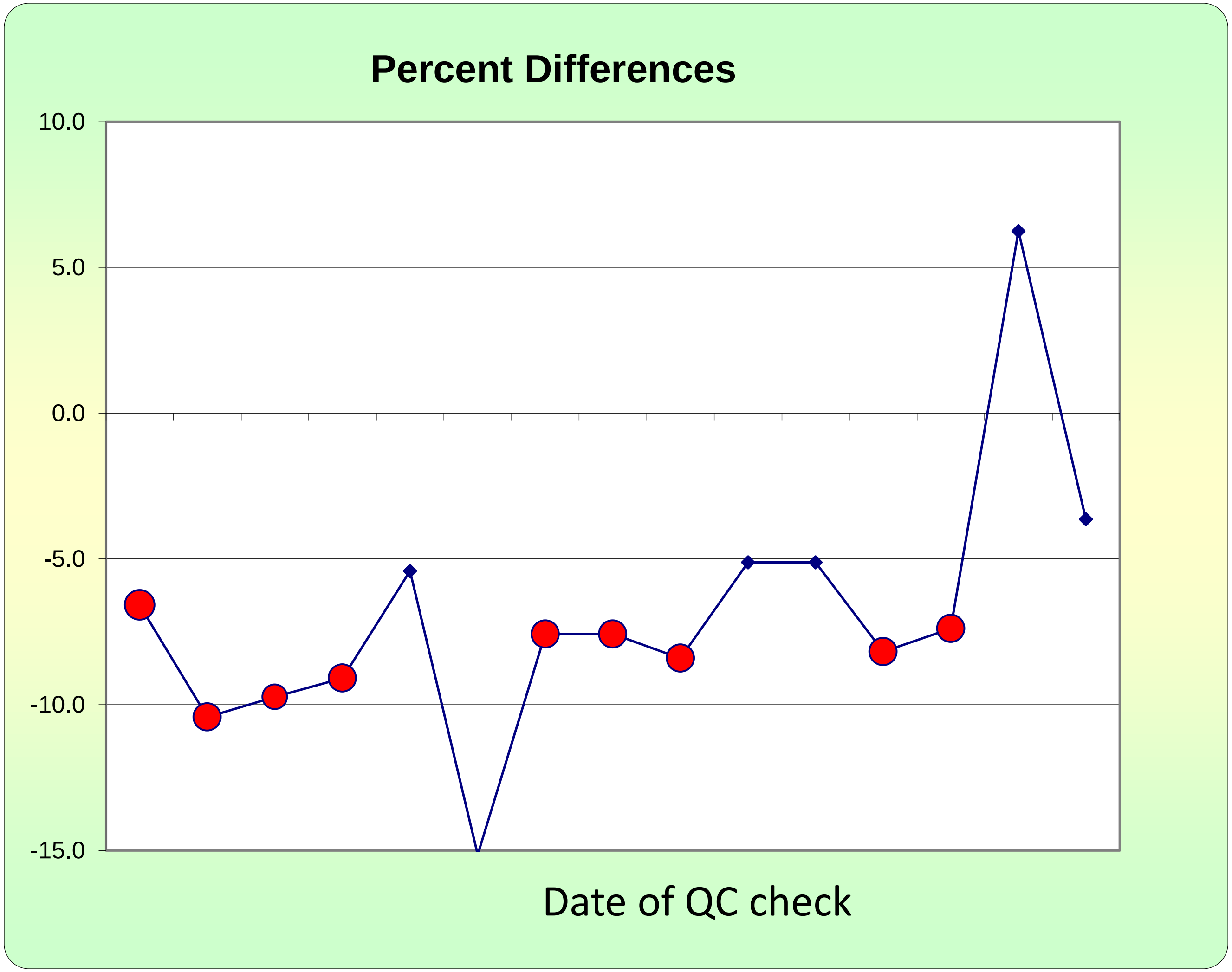
Thanks Shelly Eberly!

Bias:

- FINALLY look at where we are on the x-axis
- (Remember precision only cares about width)
- The goal for acceptable measurement uncertainty for bias is an upper 95 percent confidence limit for the absolute bias of 7 percent.



Meas Val (Y)	Audit Val (X)	d % (Eqn. 1)
85.1	91.1	-7
81.6	91.1	-10
83.4	92.4	-10
84	92.4	-9
87.4	92.4	-5
78.4	92.4	-15
85.4	92.4	-8
85.4	92.4	-8
80.6	88	-8
83.5	88	-5
83.5	88	-5
80.8	88	-8
81.5	88	-7
93.5	88	6
84.8	88	-4



Control chart from the free DASC excel spreadsheet on AMTIC

Bias statistics (CFR App A, 4.1.3):

- Remember that bias as well as precision starts from the difference between your instrument's indicated value and the known (audit) value (meas-known)/known= $\mathbf{d_i}$
- bias (jump) is calculated from $\mathbf{d_i}$
- Bias just *based on* the AVERAGE of the $\mathbf{d_i}$ with the sign taken into account (if your analyzer is always higher than the known, you have a high (+) bias

Bias in CFR eq'n 3:

$$|bias| = AB + t_{0.95,n-1} \cdot \frac{AS}{\sqrt{n}}$$

AB is the mean of the absolute values of the d_i's = **7.7**

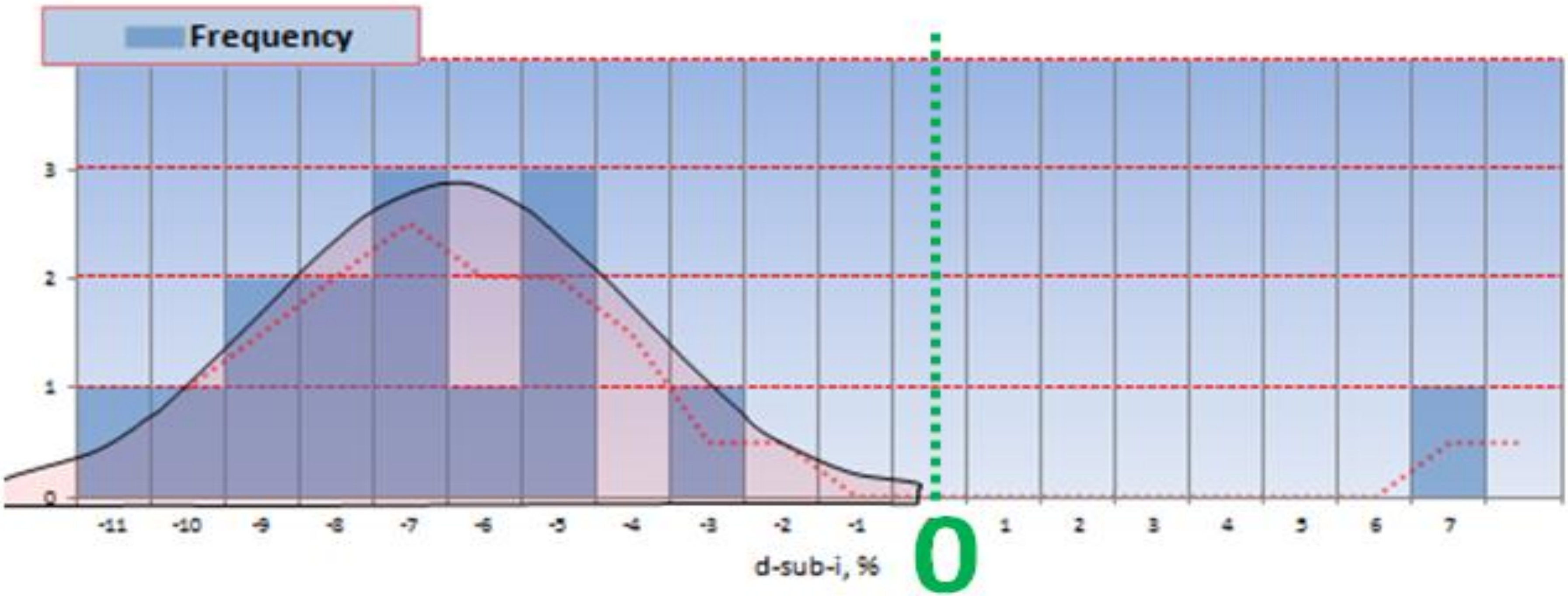
$t_{0.95,n-1}$ *is the 95th quantile of a t-distribution*
*=TINV(2*0.05,n-1) =* **1.76**

AS is the STDEV of the abs value of these d_i's = **2.78**

So
Abs value of bias = 7.7 + 1.76 * (2.78/sqrt of n)
= 8.98

d % (Eqn. 1)
-7
-10
-10
-9
-5
-15
-8
-8
-8
-5
-5
-8
-7
6
-4

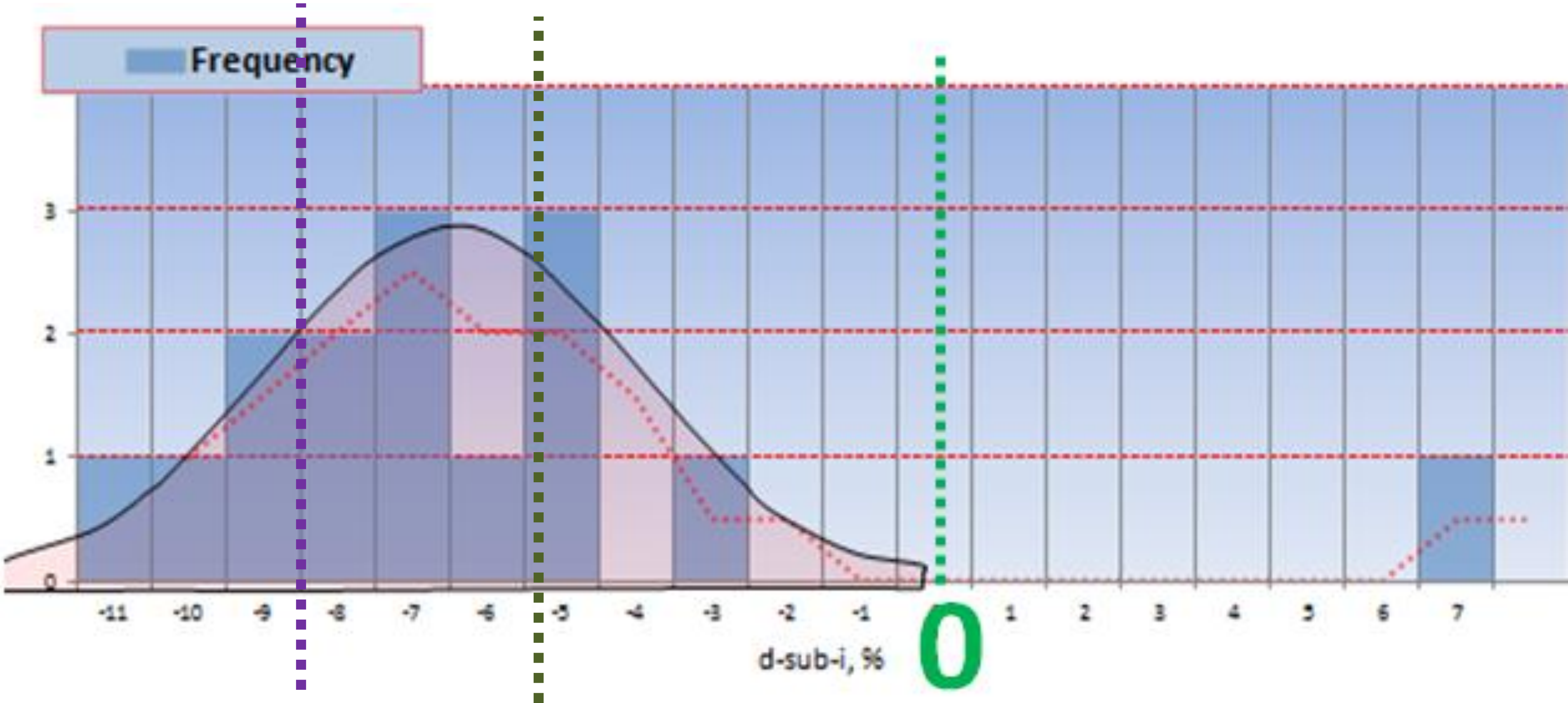
That 8.98 is the abs value of bias, now what's its sign?



- Look at 25% quartile and 75% quartile
- If they straddle zero, bias is unsigned
- If they're both negative, bias is negative
- If they're both positive, bias is positive

Quartiles?

- **=QUARTILE(d-sub-i,1) = 25% quartile = -9**
- **=QUARTILE(d-sub-i,3) = 75% quartile = -5**



Sign of Bias:

- Both quartiles are negative
- Bias is negative 8.98 = **-8.98**
- Agrees with DASC:

O_3 Assessments

Pollutant type: O_3

d (Eqn. 1)	25th Percentile	d^2	|d|	$\|d\|^2$
-6.586	-8.750	43.378	6.586	43.378
-10.428	**75th Percentile**	108.745	10.428	108.745
-9.740	-5.262	94.873	9.740	94.873
-9.091		82.645	9.091	82.645
-5.411		29.282	5.411	29.282
-15.152		229.568	15.152	229.568
-7.576		57.392	7.576	57.392
-7.576		57.392	7.576	57.392
-8.409		70.713	8.409	70.713
-5.114		26.149	5.114	26.149
-5.114		26.149	5.114	26.149
-8.182		66.942	8.182	66.942
-7.386		54.558	7.386	54.558
6.250		39.063	6.250	39.063
-3.636		13.223	3.636	13.223

CV_{ub} (%) | Bias (%)

n	S_d	S_{d2}	$\Sigma\|d\|$	"AB" (Eqn 4)
15	4.557	52.464	115.651	7.710
n-1	**Σd**	**Σd^2**	**$\Sigma\|d\|^2$**	**"AS" (Eqn 5)**
14	-103.151	1000.072	1000.072	2.783

Bias (%) (Eqn 3)	Both Signs Positive
8.98	FALSE
Signed Bias (%)	Both Signs Negative
-8.98	TRUE

CV (%) (Eqn 2)
6.11

Upper Probability Limit	Lower Probability Limit
2.06	-15.81

DASC bias in cell k13:

O_3 Assessments

	20	Pollutant type: O_3	
as Val	it Val	(Eqn. 1	25th Percentile
85.1	91.1	-6.586	**-8.750**
81.6	91.1	-10.428	75th Percentile
83.4	92.4	-9.740	**-5.262**
84	92.4	-9.091	
87.4	92.4	-5.411	
78.4	92.4	-15.152	
85.4	92.4	-7.576	
85.4	92.4	-7.576	
80.6	88	-8.409	
83.5	88	-5.114	
83.5	88	-5.114	
80.8	88	-8.182	

Bias (%)

"AB" (Eqn 4)	7.710
"AS" (Eqn 5)	2.783

Bias (%) (Eqn 3)	Both Signs Positive
8.98	FALSE
Signed Bias (%)	Both Signs Negative
-8.98	TRUE

Does this match AQS standard report AMP256 ?:

DATA QUALITY INDICATOR REPORT

One Point Quality Control

Jun. 16, 2014

PQAO:

App A? Y

POC	MT	Begin Date	End Date	# Required	# Observation	% Complete	CV UB	Bias UB
1	S	01-APR-12	31-OCT-12	15	15	100	6.11	- 8.98

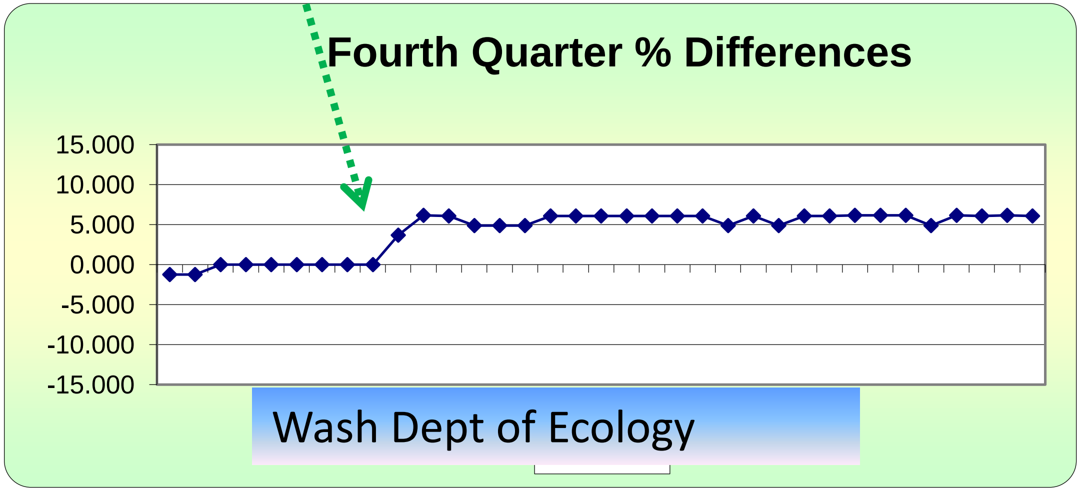
Bias UB *(upper bound of bias)* = -8.98

(goal is upper 95 percent confidence limit for the absolute bias of 7 percent)

Both bias and precision are in the same sheet (O3 P&B) in the DASC and use the same input:

Meas Val (Y)	Audit Val (X)	d_i (Eqn. 1)
0.08	0.081	-1.2
0.08	0.081	-1.2
0.081	0.081	0.0
0.081	0.081	0.0
0.081	0.081	0.0
0.081	0.081	0.0
0.081	0.081	0.0
0.081	0.081	0.0
0.081	0.081	0.0
0.084	0.081	3.7
0.086	0.081	6.2
0.087	0.082	6.1

YOU can calculate Bias over any time period using DASC

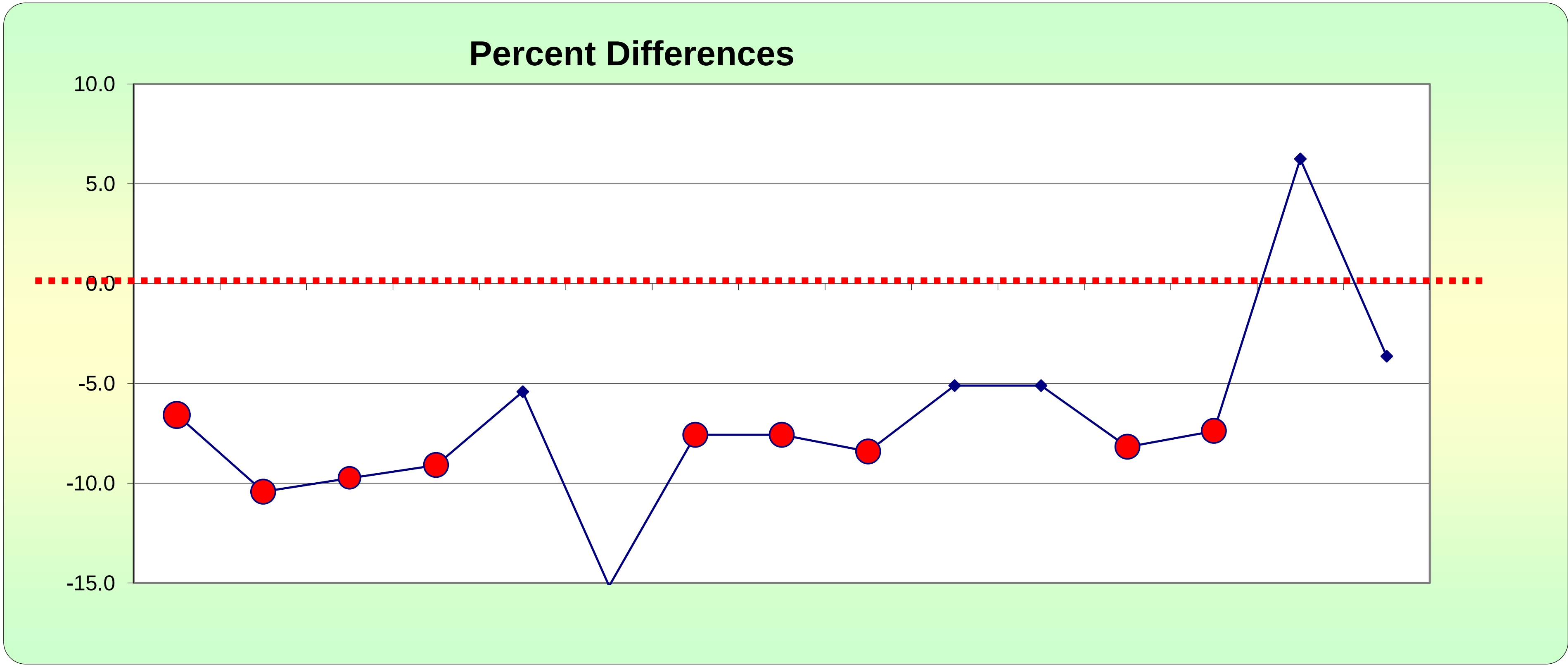


Summary of gas bias:

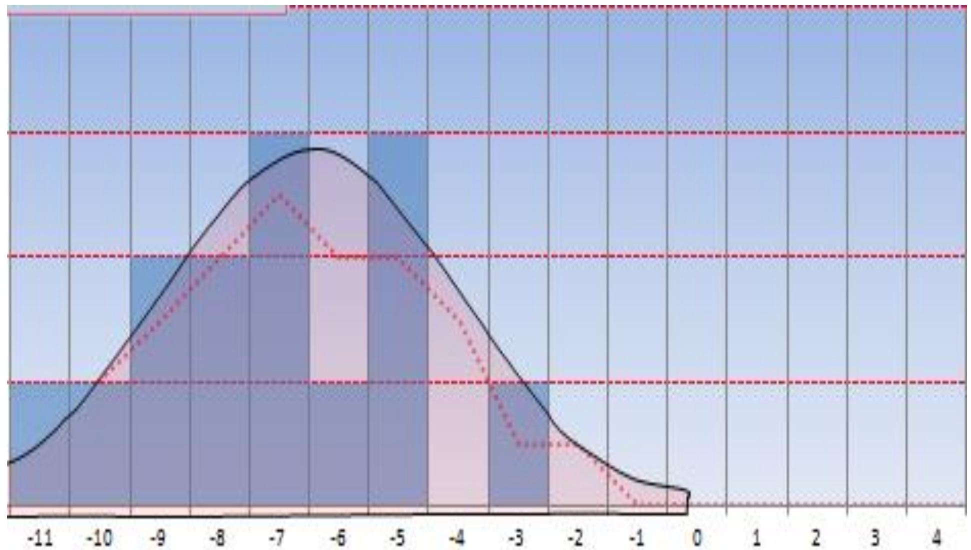
- Calculated from routine QC checks d_i
- Overall upper limit of **bias** calculated from d_i
- Then look at the sign (and the chart) for whether your analyzer is biased high (+) or low (-)
- We are 95% confident that our 03 bias is less extreme than -9%

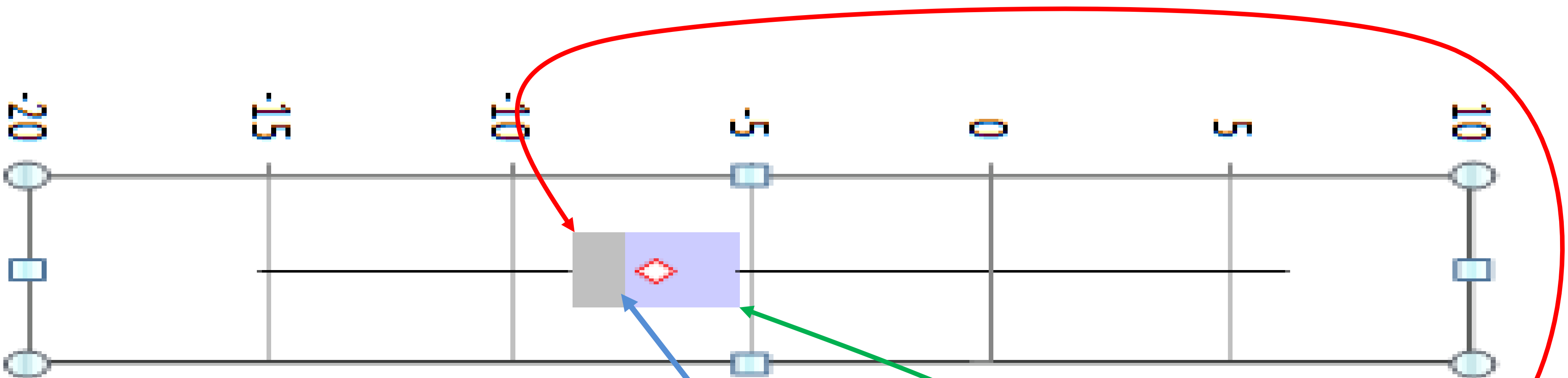
Do I invalidate pollutant data based on d-sub-i?

- Validation tables in QA Handbook:
  - Critical Measurement Quality Objective O3=7%
  - See the Data Certification ppt, next up.



Date of QC check





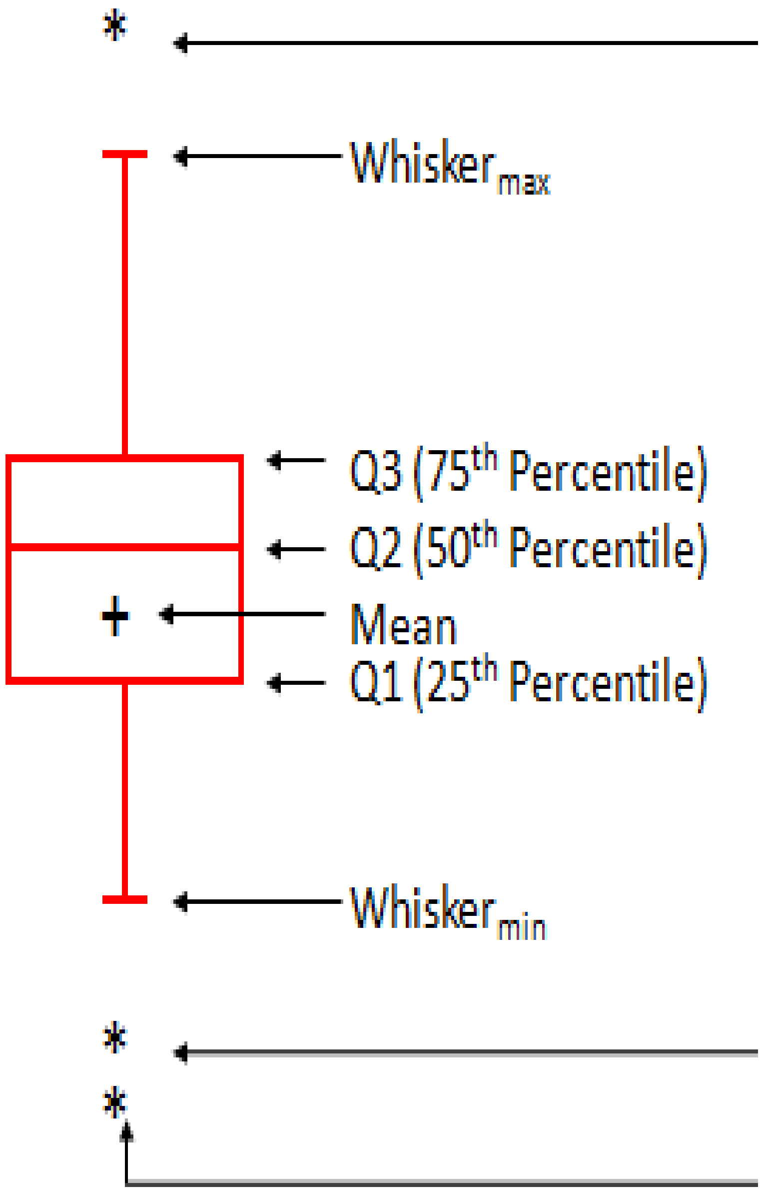
Median = 50% percentile = -7.6

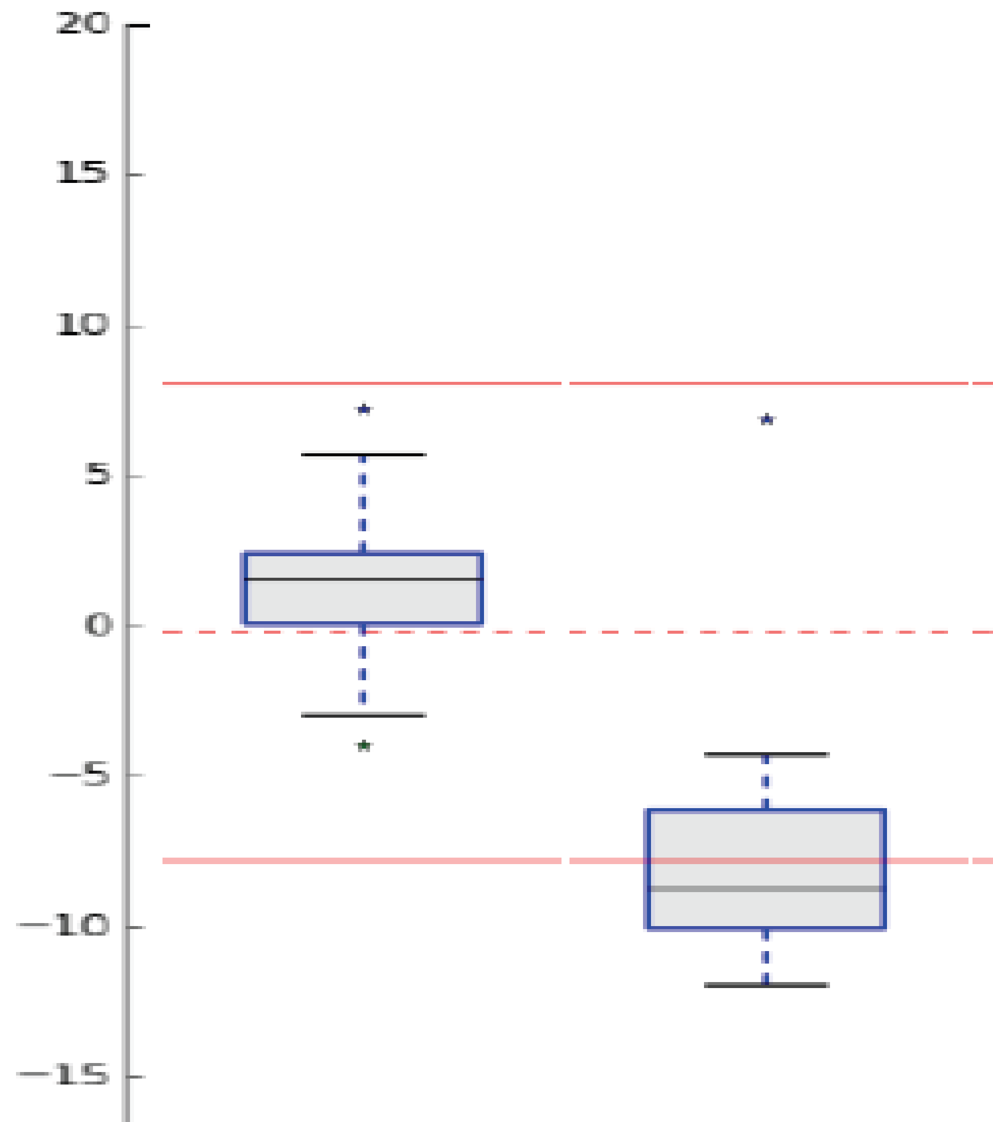
25% percentile= -8.8

75% percentile = -5.3

Mean = -6.9

CV	2.56	6.11
Bias	+2.44	-8.98
# Obs	31	15
Method	047	047





$PM_{2.5}$ Precision

- PM2.5 is the same as gaseous, except:
  - d-sub-i are from COLLOCATED, and the known is the average of the two PM2.5, so d-sub-i is
  - (RO-CO)/(avg of RO & CO)
  - Because the known is the avg of 2 measurements, add **SQRT(2)** to the denominator (divide by best estimate of truth)

STDEV

$$CV\_ub = \sqrt{\frac{n \cdot \sum_{i=1}^{n} d_i^{\,2} - \left(\sum_{i=1}^{n} d_i\right)^2}{2n(n-1)}} \cdot \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

That's the only difference in the precision stat from gas stats

$PM_{2.5}$ Bias

- PM2.5 bias same as gaseous, except:
  - **known = PEP** audit filter results, so the d-sub-i is the (field-PEP)/PEP
  - Don't take abs value of the d-sub-i
  - D is avg of these d-sub-i values
  - n is # of PEP audits, and if n=3 then t=2.9
    - (as n grows, t goes to 1.65)
  - Use the 25% and 75% quartiles → + or -

Stnd error

$$\text{Upper 90\% Confidence Interval} = D + t_{0.95,df} \cdot \frac{s_d}{\sqrt{n_j}}$$

And lower confidence interval is D minus t*stnd error

PM10 statistics:

- Bias confidence intervals based on monthly flow rate (FR) checks:
  - d-sub-i from FR
  - THEN bias statistics are the same as PM2.5
- Flow rate “acceptability” limits are based on 6-month FR audits (with FR audit device not the same one you use for the monthly):
  - Limit = D +- 1.96 * STDEV

d-sub-i = (sampler-audit_FR)/audit_FR
and D is their average

Thank you!

- Work with Tribal Air Agencies
- Knowledge = Power; Let's Share
- Melinda Ronca-Battista melinda.ronca-battista@nau.edu; this presentation is on our YouTube channel